Numerical Calculation of the Neutron Wave Packet Interaction with an Oscillating Potential Barrier

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Abstract

It is assumed that in neutron optics the concept of an effective potential has a limited range of applicability at the accelerations of matter less than a certain critical value. The experiment intended to study the interaction of a neutron wave with matter moving with acceleration higher than the critical one was proposed. In this paper, in the framework of the proposed experiment, numerical calculations of the passage of a wave packet through the oscillating in space interference filter were carried out. The calculations were based on the assumption of the potential dispersion law validity.

1. Introduction

It is known that the theory of refractive index is valid for neutron waves, as well as for waves of a different nature. The physical nature of the refractive index is due to the interference of the incident wave and waves scattered by elementary scatterers in matter [1].

This interaction can be described by introducing an effective potential. The main contribution to neutron scattering in the medium is made by nuclei. The exact form of the strong interaction potential is unknown. However, since the wavelength of slow neutrons is much larger than the size of a nucleus, when calculating the scattering cross section, the radius of the nuclear interaction can be neglected and the potential describing the point interaction can be considered [2]. This is the so-called Fermi "pseudo-potential":

$$U(\vec{r})=\frac{\hbar^2}{2\pi m}b\delta(\vec{r}-\vec{r}_0) \quad (1)$$

The quantity b is the coherent scattering length and is determined from the scattering cross section of slow neutrons $\sigma_{scat}=4\pi b^2$.

For a slab with a nucleus density ρ, the averaging of the "pseudo-potential" with respect to the volume gives the following expression:

$$V=\rho\int U(\vec{r})d^3r=\frac{\hbar^2}{2\pi m}\rho b. \quad (2)$$

The expression for the refractive index of a neutron wave in matter is written as follows [3]:

$$n^2=1-\lambda^2\frac{2m}{\hbar^2}V=1-\frac{4\pi\rho b}{k_0^2}. \quad (3)$$

Formulas (2) and (3) are equivalent to each other.

The legitimacy of using the concept of "effective potential" or an equivalent formula (3) for describing the optical properties of a uniformly moving medium is beyond argument due to the validity of the Galilean transformation for the wave function of a non-relativistic particle [4]. This motion affects only the value of the phase of the wave that has passed through the sample of matter. Neutron optics of moving media is described in [5-12].

The situation changes in case of accelerating motion of matter. It was found that in this case the frequency of the wave passing through the sample differs from the frequency of the incident wave [13, 14]. Based on the assumption of the validity of the potential dispersion law for accelerated motion of matter, it was shown that when the neutron escapes from the plate the neutron energy differs from the initial energy by an amount of

$$\Delta E \cong mwd\frac{1-n}{n}. \tag{4}$$

Here, m is the neutron mass, w is the plate acceleration directed along the neutron velocity, d is the plate thickness, and n is the refractive index of the plate material.

The first report on the experimental observation of the change in the ultracold neutron energy, when passing through the accelerating sample, appeared in 2006 [15], and the results of a more detailed study of the accelerating substance effect were published in [16]. The results of these experiments, in which the acceleration of the sample reached 75 m/s^2, were in good agreement with the theoretical predictions. It should be emphasized that the theory was based on an in non evident assumption of the validity of the potential dispersion law.

The question of the applicability of an "effective potential" for describing the optical properties of matter for all values of matter acceleration apparently remains open. The point is that in the theory of dispersion, which is, in fact, the theory of multiple scattering of waves, the assumption of the sphericity of the interfering scattered waves is rather significant. At the same time, in the non-inertial frame of reference associated with the accelerating substance, the idea of spherical waves is wrong and this can affect the condition of their interference.

This circumstance was pointed out in [16, 17], and a more detailed discussion of this problem was presented in [18]. Estimates of matter acceleration were made. At such estimates deviation from the potential dispersion law is possible by an amount of the same order as the phenomenon itself. For the case of ultracold neutrons (E = 100 neV), the value of the critical acceleration is $w_c = 8\cdot 10^5\ m/s^2$. This acceleration is achievable in laboratory experiments.

Although the law of neutron wave dispersion in a substance moving with a very high acceleration is unknown, the information can be obtained from the experiment [19]. The experimental strategy of such investigation is as follows. It is planned to conduct two experiments to observe the interaction of neutrons with a potential oscillating in space. In one of them, the acceleration of the sample is less than the critical one, while in the other it exceeds the critical value. In both cases, the results are compared with a quantum calculation based on the assumption of the validity of the concept of effective potential. Obviously, to implement such a program, it is necessary to have software-mathematical tools for quantum calculations. In this paper, calculations of the wave packet passage through an oscillating interference filter were made.

2. Envisaged experimental implementation

Considering different possibilities of setting up the experiment, an experiment on the neutron wave passage through an oscillating interference filter was chosen. Such an experimental setting has the following advantage: the transmitted wave is time-modulated because of a periodic change in the neutron energy in the coordinate system of the moving filter. This makes it possible to abandon a spectrometric experiment by starting to register the time oscillation of the stream that has passed through the sample. The disadvantage of this type of experiment is the limitation of the possible oscillation frequency, since the lifetime of the resonance state in the filter and, correspondingly, the tunneling time, are of the order of 10^{-7}*sec* [20, 21].

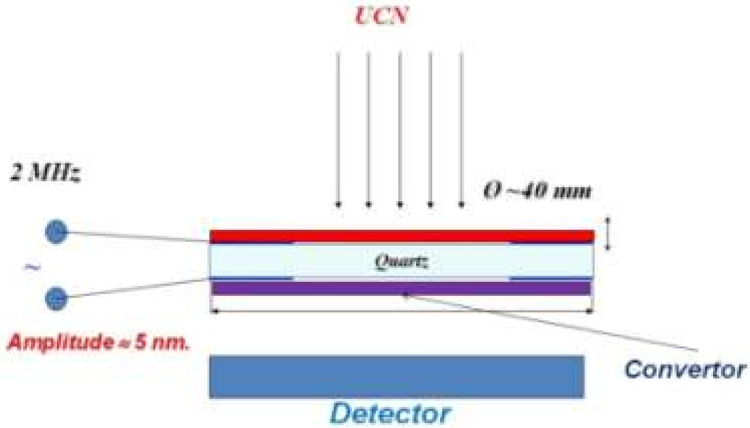

Fig.1. Scheme of the experiment on verification of the potential dispersion law for a substance in strongly non-inertial frames of reference.

A possible experimental realization of this study is illustrated in Fig.1. Three thin slabs forming a potential structure are applied to a quartz plate that acts as a resonant piezo driver [15]. On both surfaces of the plate, a thin aluminum foil serving as electrodes is preliminarily applied. Ultrasonic vibrations of the plate are excited when an alternating voltage is applied to the electrodes. The thickness of the plate should be equal to or multiples of half the length of the ultrasonic wave. For operation at a frequency of 2 *MHz*, it should be of the order of 0.3 *mm*. Such a quartz plate allows UCN to pass through sufficiently well. It is easy to estimate that the high-frequency oscillations of the flow that arise when the filter moves quickly disappear with distance because of the dispersion of the velocities. Therefore, the neutron detector should be as close as possible to the filter. It is assumed that this problem will be solved by applying to the exit surface of the plate a thin (0.2 μm) layer of the ^{10}B isotope converting a neutron flux into an α-particle flux as a result of the $^{10}B(n,\alpha)^{7}Li$ reaction. α-particles, which have a subluminal velocity, are detected by a semiconductor silicon detector located near the converter.

As a filter, it is planned to use neutron interference filters, which are quantum analogs of Fabry-Perot interferometers (Fig. 2). In the simplest case, the filter is three slabs of two kinds of matter deposited on a substrate transparent to neutrons. The materials of the layers are chosen in a way that the effective potential of the outer layers $V = \frac{\hbar^2}{2\pi m}\rho b$ considerably exceeds that for the inner slab and the substrate. Thus, the potential structure of the filter is two barriers with a well between them. With the parameters chosen in a certain way in the well region, a “quasibound” state can form, and the structure transmission function has a pronounced peak of resonant transmission at the energies corresponding to the position of the level of the “quasibound” state. The transmission function of such a structure can be found on the basis of the solution of the boundary-value problem, that is assuming the continuity of the wave functions and their derivatives at all interfaces.

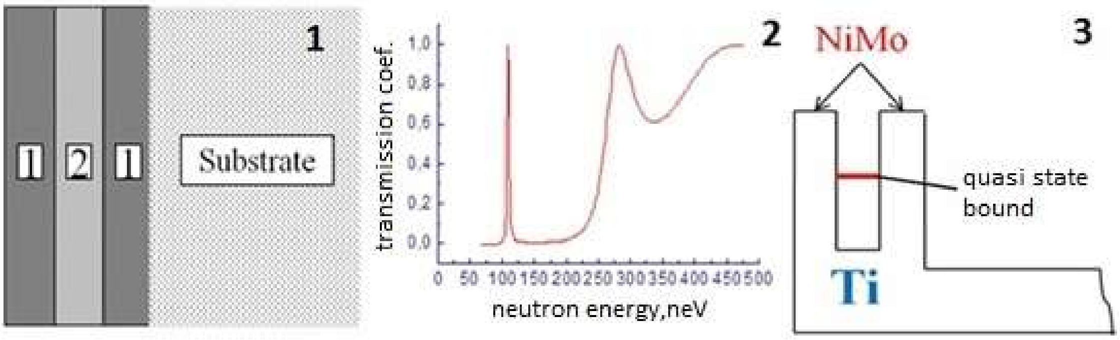

Fig. 2. Neutron interference filter. (1) is a schematic diagram of the simplest filter, (2) is the filter transmission function, (3) is the potential structure of the filter.

3. Interaction of neutrons with a potential barrier oscillating in space

The time evolution of a wave packet is described by a non-stationary Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=\hat{H}(t)\Psi(x,t). \tag{5}$$

The initial wave function was defined as follows:

$$\Psi_0(x,0)=\frac{\sqrt{\delta_p/\hbar}}{\sqrt[4]{\pi}}\exp(-ikx)\exp\left(-\frac{(x-x_0)^2}{2\delta_x^2}\right), \tag{6}$$

where δ_p is the width of the wave packet in the momentum space, δ_x is the width of the wave packet in the coordinate space, and k is the initial wave number of the neutron.
The potential $V(x, t)$ is bounded by a finite region, it is given by the expression:

$$V(x,t)=\bar{V}\left[x-A\cos(\omega t+\varphi)\right], \tag{7}$$

where $\bar{V}(x)$, in general, is any potential structure moving as a single whole:

$$\bar{V}(x)=\begin{cases}V_0(\xi), & 0\le x\le L\\ 0, & For\ other\ \ space\end{cases}. \tag{8}$$

Here $V_0(\xi)$ determines the internal structure of the potential.

There are many methods for numerical solution of the non-stationary Schrödinger equation. To solve this problem, the splitting method of the evolution operator was used [22].

Numerical calculation was performed for a three-layer filter consisting of layers of *NiMo*, *TiZr*, *NiMo*, being 29.5, 23, 29.5 nm thick. The values of the effective potentials for these two materials are 226 and 0.26 neV. For simplicity, the substrate potential was assumed to be zero. In the numerical solution, the width of the wave packet was δE = 1 neV, the time step dt = 1 nsec, the discretization step of space dx = 4 nm.

This solution is compared with the classical solution based on the continuity equations, obtained as follows. For a plane wave, the recurrent method of Parrath [23] allowed calculating the transmission of a three-layer structure as a function of the plane wave energy, and its convolution was found with a spectrum corresponding to the parameters of the wave packet used by our program. A comparison of the results obtained by the two methods is illustrated in Fig. 3.

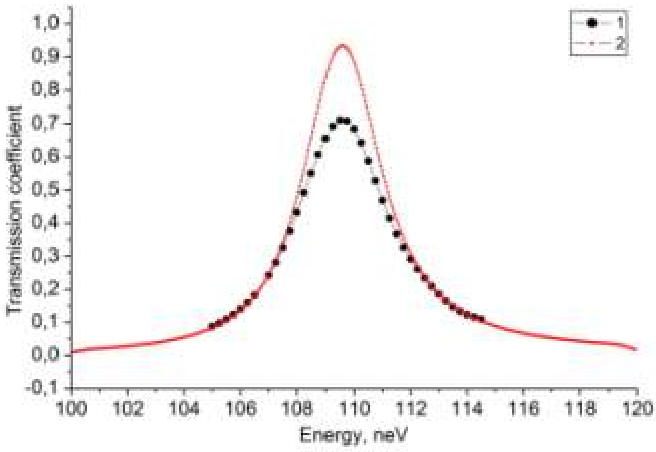

Fig.3. Interference filter transmission function obtained by two methods 1) Step-by-step numerical solution based on the splitting method of the evolution operator, 2) Solution of the boundary value problem.

The difference between the results can be explained by the presence of discretization in the coordinate and time, leading to some uncertainty in the position of the boundaries of the filter layers. It is known that the position of the resonance is very sensitive to the width of the well formed by two barriers. Fluctuations in the position of the barriers lead to line blurring, degrading the transmission characteristics.

The width of the wave packet was chosen in such a way that the transit time of the packet through the filter was much greater than the period of the oscillations. The restriction on the width of the wave packet is also imposed by the fact that the narrower the wave packet in the impulse representation is, the more space it occupies and the more time it takes to calculate. In the calculation, the width was assumed to be $\delta E = 1$ *neV*. A numerical calculation was made for the oscillation regime with a frequency of 2 *MHz* and amplitude of 5 *nm*.
The results of numerical calculations of the wave packet shape in the coordinate representation due to the intensity oscillation, as well as the spectra of the transmitted and reflected states, are given below. The wave packet evolution over time is shown in Figure 6.

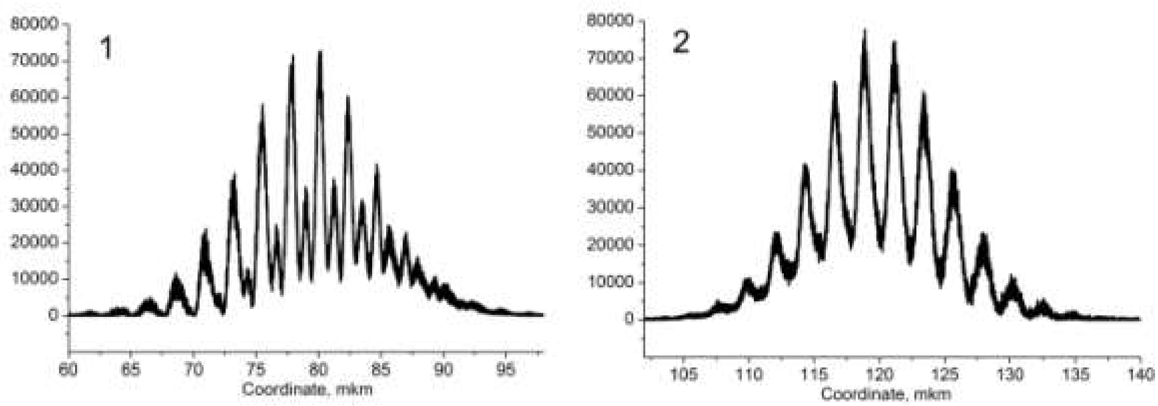

Fig. 4. Wave packets that were reflected (1) and that penetrated through (2).

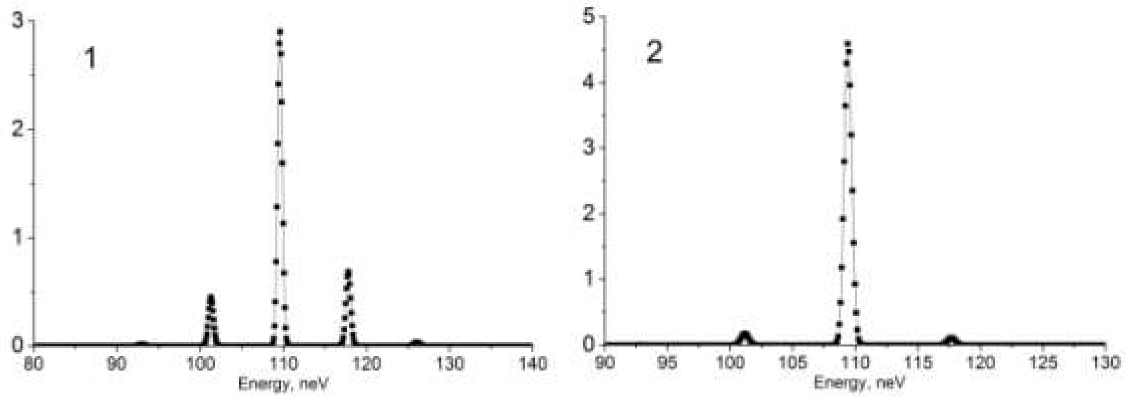

Fig. 5. Energy spectrum of the reflected (1) and transmitted (2) states of the wave function.

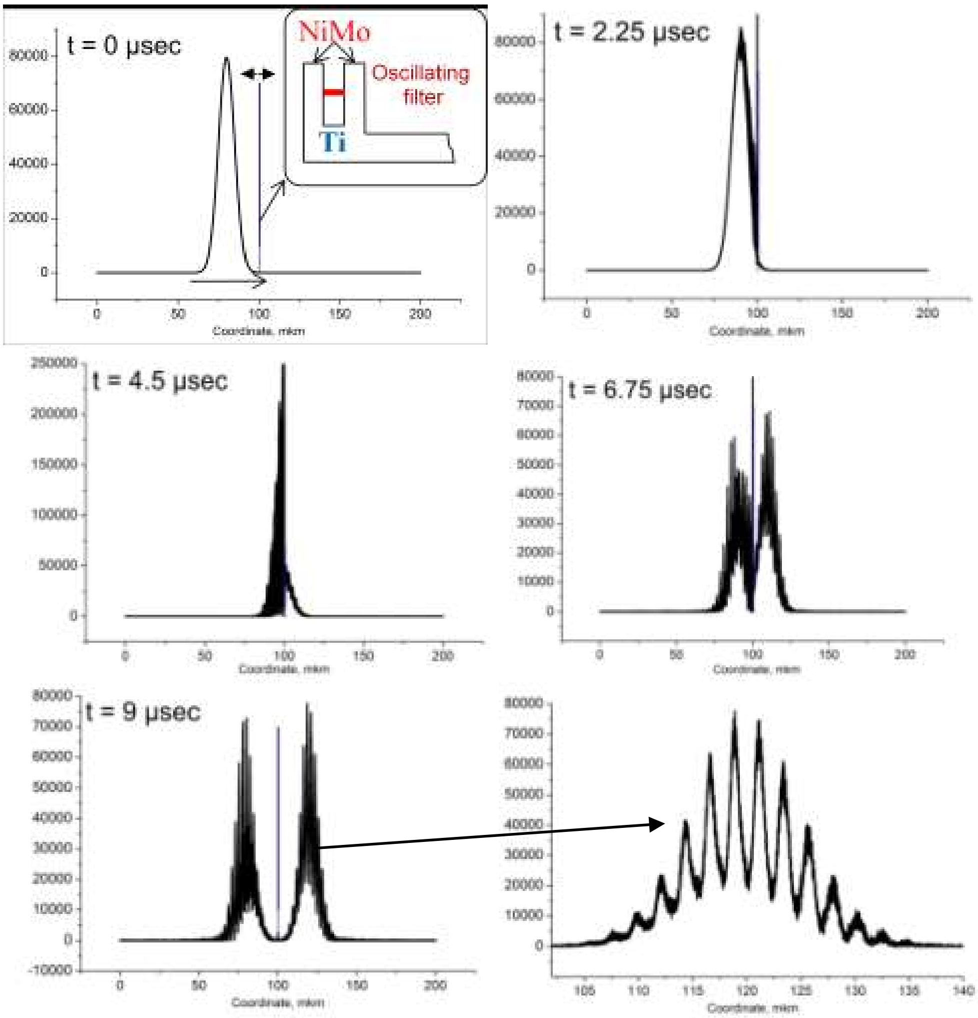

Fig. 6. Wave packet evolution in time when being reflected and passing through an oscillating interference filter.

4. Conclusion

The above-given result requires reflection and analysis. The fact is that, from general considerations, one should expect that the oscillation frequency of the stream should be twice as large as the spatial oscillation frequency of the filter, since the maximum transmission corresponds to the stopping times, that is, twice per period. However, the results of the calculation suggest that the frequencies of oscillations of the flow and the intensity are equal. This may be explained by a certain violation of the resonance conditions, when the scanning by the transmission line along the original spectrum occurs on the slope of the resulting function and does not capture the maximum. This may be due to a relatively large step in the coordinate $dx = 3$ *nm*, which is eroding the boundaries of the filter layers in the calculation. If this assumption is correct, the obvious solution to this problem is to decrease the step both in the coordinate dx and in the time dt. However, this will require the use of other hardware and other software. This task is a subject of future work.

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